

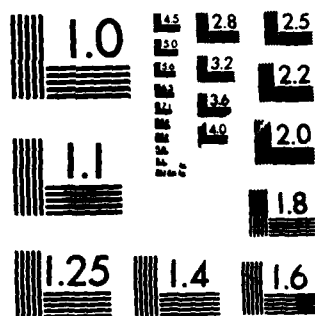
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PURCHASE OF A VAX 11/750 COMPUTER(U) NORTH DAKOTA STATE 1/1
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PURCHASE OF A VAX 11/750 COMPUTER

FINAL REPORT

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The VAX 11/750 was purchased from Digital Electronics in the Spring of 1985. According to our benchmarks using GAUSSIAN82 and GAMESS, the VAX throughput is approximately 1/13th of an IBM 3081. The reliability of the computer has been excellent. In the approximately 18 months since the computer was obtained, there has been virtually no down time, except for that caused by air conditioning failure or to install software updates. This has allowed us to run jobs which require several CPU days to be completed. This would clearly be impossible on any campus machine. The system has 900 megabytes of disk storage, and the main memory has been upgraded to 8 megabytes. This allows us to perform calculations on very large molecules. Because it is so easy to use the VAX VMS operating system, nearly all of our program development is performed on the VAX. This includes improvements in GAMESS and GAUSSIAN82, as well as development of new programs. Particular projects to which the VAX has been applied include:

1. Evaluation of Pi Bond Energies. Using MCSCF wavefunctions and the 3-21G(d) basis set, we have evaluated the strength of the pi bonds in $H_nA=BH_m$ compounds, with A, B = C, N, Si, and P. This is accomplished by rotating each molecule about the AB bond, thereby breaking the pi bond. We find that the abilities of C and N to form pi bonds are approximately equal, while that of P is much smaller and that of Si is smaller still. A paper (M.W. Schmidt and M.S. Gordon) on this work will be submitted shortly to the Journal of the American Chemical Society.

2. Phosphorus Clusters. An earlier semi-empirical paper had concluded that cubic P_8 is stable relative to two tetragonal P_4 molecules, even though this appeared to be contrary to available experimental evidence. Our ab initio calculations, including second order perturbation theory (MP2) corrections, predict P_8 to be a minimum on the potential energy surface, but, in agreement with experiment, much less stable than two P_4 's. This work has been published (M.W. Schmidt and M.S. Gordon, Inorg. Chem.,

3. Highly Strained Ring Compounds. We have embarked on a systematic investigation of strained rings containing one or more silicon atoms and their carbon analogs. The VAX has been used to study a series of bicyclobutanes containing 0-4 silicon atoms, and their unsaturated monocyclic analogs. The most unusual structures occur in the compounds with two silicons. When the bridge bond is CC, the CC bond length is 1.75A, to our knowledge the longest CC bond known. On the other hand, in an isomeric structure the bridging SiSi bond is 2.11A. This is shorter than a typical silicon-silicon double bond! However, when the curved nature of this bond is taken into account, it lengthens considerably. In most cases, the monocyclic isomers are more stable, but this is not so for the tetrasil species. We are now proceeding to evaluate the ring strain in these compounds, as well as their heats of formation.

4. Basis Sets. As the first step in developing improved basis sets for main group elements, we have been evaluating existing basis sets for these atoms. We have systematically compared Hehre's STO-3G and Huzinaga's MINI basis sets for 3rd, 4th, and 5th period main group elements by calculating geometries for small molecules containing these elements. When MINI is properly scaled, it produces geometries which are more accurate than those from STO-3G in a least squares sense. However, the difference between the accuracy of these two minimal basis sets is probably not enough to offset the greater efficiency of STO-3G. At the other end of the spectrum, we have predicted the heats of formation of simple

third period hydrides using the McLean-Chandler basis sets and fourth order perturbation theory. The rms error in predicted heats of formation is only 4 kcal/mol. This is better than the triple zeta basis set used by Pople and co-workers for the analogous second period hydrides. These results have just been submitted to J. Phys. Chem. (M.S. Gordon and J. Heitzinger)

5. Population Analysis. Weinhold has recently developed an alternative to the Mulliken population analysis, using natural atomic orbitals. The new procedure has been tested on our VAX by systematically analyzing AH_n , closed shells and radicals, AH_{n-1}^+ cations and AH_{n-1}^- anions. Preliminary results suggest that the basis set dependence of the new analysis is much more stable than that for the Mulliken analysis.

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